

REMARKS

At the outset, the Applicant wishes to thank Supervisory Patent Examiner (SPE) Jerry A. Lorengo and Patent Examiner Jennine M. Brown for the many courtesies extended to Dr. Sonke Lorenz, and to the undersigned attorney, during the Personal Interview on December 13, 2005, at the U.S.P.T.O. The substance of this Personal Interview is set forth in the Examiner Interview Summary, and in this Amendment.

During the Personal Interview, it was indicated that a certified English translation of the priority document would be filed. Thus, this document is now being filed, and is enclosed herewith. The Applicant claims all benefits under 35 U.S.C. 119, to which he is entitled.

During the Personal Interview, there was a discussion of various objections to claim language that have now been overcome due to the modified terminology of new claim 19 which replaces claim 17, which was cancelled.

Hence, objected to terms such as "arbitrarily or randomly," or "crossing" and "mutation" have now been cancelled and do not appear in new claim 19.

Also, during the Personal Interview there was a discussion of the general inventive concept of the present invention, along with specific limitations set forth in claim 17, and how this was clearly illustrated in the Specification and specifically in the Examples in the Specification. Then there was also a discussion of new claim 19, which is a version of claim 17 that was written so as to reduce the total number of steps present in the claimed invention without adding any new matter to the present patent application. Specifically, the preamble of claim 19, has the language "selecting components for the preparation of" cancelled and replaced by the word "producing."

Then, in step (b), the clause "wherein n is finite" has been added. In step (c), the word "computerized" is added before the phrase "random-number generator." These terms were discussed during the Personal Interview.

For all these reasons, it is firmly believed that the Specification, and all the claims are in complete compliance with all the requirements of 35 U.S.C. 112. Withdrawal of this ground of rejection is respectfully requested.

The Applicant comments upon the prior art rejections of the

claims as follows.

The present application specifies a genetic algorithm for selecting components for the preparation of solid catalysts. In particular a method for producing active and/or selective solid catalysts of inorganic or organometallic materials or mixtures thereof is claimed in the newly presented claim 19, comprising the steps of:

- (a) preparing a first generation of catalysts and measuring the "fitness" of the first generation catalysts according to the activity or selectivity or activity and selectivity;
- (b) selecting the best catalysts from all previous generations;
- (c) preparing the next generation from the selected catalysts in step (b) by exchanging randomly selected components between randomly selected catalysts; and/or randomly varying the mole amounts of randomly selected components of randomly selected catalysts;
- (d) determining the fitness of the new generation experimentally;
- (e) returning to step (b) until the fitness does not significantly increase any more.

The method for producing catalysts employs an iterative, directed optimization of the previously generated catalysts using the principles of a genetic algorithm.

Kudo (U.S. Patent No. 3,929,670) discloses a specific catalyst for reducing nitrogen oxides. No optimization of a group of catalysts is disclosed by *Kudo*.

Inoue et al. (U.S. Patent No. 6,110,860) discloses a specific catalyst for exhaust gas purification. No optimization of a group of catalysts is disclosed by *Inoue*.

Schultz et al. (U.S. Patent No. 6,420,179) discloses a method and apparatus for the preparation and use of a substrate having an array of diverse materials in predefined regions thereon. The invention is directed to combinatorial chemistry as disclosed in the prior art discussion of the present application. A library of a number of different molecules on a substrate is being built using the principles of combinatorics, i.e. all possible permutations of the selected components are being synthesized and measured.

Since all possible permutations of the components are synthesized, an array of catalysts as disclosed by *Schultz* can

consist of more than 10^6 different inorganic compounds (col. 4, lines 35-51). The present invention allows finding better catalysts while preparing only a small number of catalysts as shown by the examples. In contrast to the present invention, Schultz does not disclose an optimization step. No iterative optimization is performed.

Cawse (U.S. Patent No. 6,728,641) discloses a method and system for selecting a best case set of factors for a chemical reaction. The invention by *Cawse* uses combinatorial high throughput screening. Again, as in the invention by *Schultz et al.*, *Cawse* uses the principles of combinatorics to generate a vast amount of samples, i.e. all possible n-tuple combinations of the factors are generated (col. 4, lines 47-65).

In contrast to the present invention, no iterative optimization is performed. In particular, no selection of the best catalysts, no modification of the catalysts by exchange of components and/or variation of components amounts is disclosed.

Deem et al. (U.S. Patent No. 6,640,191) discloses methods for generating multiple rounds of combinatorial libraries, which use Monte Carlo methods to search the multi-dimensional composition space of combinatorial chemistry.

A first generation of catalysts is generated. The values of the set of samples are changed by a Monte Carlo selection method, which is profoundly different from the Genetic Algorithm approach of the present invention.

In particular, the values of the variables are randomly changed only a small amount, i.e. the composition space is sampled in a very slow manner in contrast to the present invention, where the variation of the mole amounts is not restricted to be small. Furthermore, *Deem* modifies each current sample, wherein the present invention varies only randomly selected components of randomly selected catalysts. A Monte Carlo probability proportional to $\exp(\beta E)$ is used by *Deem* for the selection, where E is the figure of merit is used in the selection and β is an adjustable parameter. Note that the present

invention does not rely on an adjustable parameter to perform the selection. Moreover, the Monte Carlo selection probability differs from the selection probabilities in step (c) of the present invention.

In addition, an exchange of components as claimed in step (c) of the present invention is not at all discussed by Deem. An exchange is only presented as a step of a parallel tempering mechanism for two different sets of samples of one generation. Whole catalysts are swapped between two sets of samples of the same generation, wherein both sets of samples use a different parameter β (col. 10, lines 12-24). Parallel tempering is related to the fact that Deem uses a Monte Carlo selection with a parameter β , which is physically related to the temperature ($\beta=1/T$) (see Deem, col. 7, line 2). The concept of parallel tempering is well known in the art of optimization theory. It is used to escape from local maxima and not for an improvement of the sampling of configuration space itself. Parallel tempering does not form a part of the present invention. The exchange of

catalyst components between catalysts of a single set of catalysts of a present generation is not disclosed by Deem.

Subsequently, Deem measures a figure of merit experimentally. Deem then forms a modified set of samples by focusing on two catalysts of the present set of samples at a time only. A proposed individual sample replaces a current individual sample according to a detailed balance probability. If the figure of merit of the new sample is larger than the figure of merit of the old sample, the old sample is replaced. This is in sharp contrast to the present invention. In the present invention the best catalysts of all previous generations are included in the new generation. Deem focuses only on the competition of two samples of the present generation. In the present invention, if the old sample would have a higher figure of merit than most of the other samples, it would not be discarded but would remain in the set of samples. Thus, during optimization the present invention focuses on the best group of samples rather than the best individual as done by Deem et al.

Moreover, *Deem* even accepts new samples with a lower figure of merit compared to the old sample according to the Metropolis probability. In contrast to the present invention, the new sample is not compared to the other samples, i.e. even a sample with the worst figure of merit of all samples could be included in the new set of samples of *Deem*.

To summarize, *Deem* disclose a profoundly different optimization scheme for new catalysts. Neither the selection nor the modification step of the present invention is disclosed by *Deem*.

Therefore *Deem* does not anticipate the subject-matter of claim 17 as well as the newly presented claim 19.

Also, because the present patent application is entitled to rely upon its priority date of September 11, 1998, this antedates the *Cawse* reference date of January 21, 2000, or the *Deem* reference date of December 30, 1999. Thus, *Cawse* and *Deem* are not available as prior art references and should be withdrawn.

For all these reasons, none of the prior art references provide an identical disclosure of the claimed invention. Thus, the present invention is not anticipated under 35 U.S.C. 102. Withdrawal of this ground of rejection is respectfully requested.

In view of the amendments to the claims, all the claims are believed to be patentable under 35 U.S.C. 103. Withdrawal of this ground of rejection is respectfully requested.

Respectfully submitted,
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Enclosures: Certified English translation of Priority Document

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